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Quantum Monte Carlo Simulations of Strongly Correlated Electron Systems: The Dimensional Crossover

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The research carried out in this project aims to exactly solve models of correlated electron systems with large-scale fermion quantum Monte Carlo simulations. The goal is to understand the emergent many-body phenomena and critical behaviour. We will first provide an overview of themes and then concentrate on the so-called dimensional crossover phenomena. In this domain, we were able to provide dynamical information about the confinement of fractionalised spinon excitations in weakly coupled Hubbard chains. Such calculations are relevant for the understanding of neutron scattering experiments on $KCuF_3$. From the technical point of view we are using and developing a number of algorithms, including continuous-time interaction expansion and determinantal quantum Monte Carlo methods.

1 Introduction

Computational approaches to quantum matter play an important role for our understanding of experiments and theoretical models. In recent years, we have witnessed sustained progress both at the algorithmic level as well as in computational power. In some domains, quantum simulations have achieved such a degree of sophistication that they can calibrate experiments. When electronic correlations play an important role, this is possible only for those systems where simple models can account for the experimental setup. Experiments studying transport through a Kondo dot coupled to superconducting leads can be understood to amazing precision with state-of-the-art continuous-time quantum Monte Carlo (QMC) impurity solvers[1]. Advances in QMC simulations of fermions now allow to include long-range Coulomb interactions in model calculations. In the absence of screening – as appropriate for graphene – this is an important step towards realistic modelling[2]. QMC simulations of simplified models are equally important for our understanding of fundamental phenomena such as the electron-phonon interaction[3–5], metal-insulator transitions of Dirac fermions[6,7], as well as the interplay between topology and interactions[8,9]. These topics are being actively pursued in our group. In this article we will concentrate on the so-called dimensional crossover, which plays an important role in the understanding of many experiments.

The interplay between interactions and spatial dimensionality is the key to the essential physics of a large number of materials, ranging from high-temperature superconductors[10] to low-dimensional charge-transfer organic salts[11]. Dimensionality also plays a decisive role in phase transitions and critical phenomena in quantum magnets[12]. In three-dimensional (semiclassical) antiferromagnets, the spontaneous breaking of a continuous symmetry below a finite critical temperature is accompanied by gapless Goldstone modes associated with long-wavelength fluctuations of the order parameter. In contrast, quantum

antiferromagnets such as layered or one-dimensional systems do not develop long-range order at finite temperatures. Numerical simulations aimed at understanding how the semi-classical dynamics characteristic of an ordered phase crosses over to the critical dynamics of lower-dimensional quantum-disordered magnets are thus necessary to explain complex excitation spectra of real quasi-one-dimensional magnetic materials.

In the realm of the solid state, controlling dimensionality implies that the thermal energy (or frequency) is larger than the effective coupling which triggers a dimensional crossover. Under those circumstances, there is no coherence between the lower-dimensional units, so that they effectively decouple, and one can thus expect drastic changes in the physical properties of the system. The dimensional crossover is particularly interesting when elementary excitations fractionalise in the lower-dimensional limit[13]. For example, neutron scattering experiments on weakly coupled spin ladders of $CaCu_2O_3$ show the two-spinon continuum at frequencies larger than the interchain exchange and their confinement in the higher-dimensional ladder system emerging at lower energies[14]. Another experimental realisation is provided by $KCuF_3$ which consists of weakly coupled spin-1/2 chains[15]. At high frequencies one observes the two-spinon continuum, signalising free spinons. In the low-frequency limit, pairs of spinons bind to form the Goldstone mode (spin-waves) of the broken-symmetry phase. Intermediate dimensions and short-range quantum magnetism became recently accessible in ultracold atomic gases by tuning optical lattices comprising weakly coupled one-dimensional chains[16]. A variable strength of the interchain coupling allows one to study the impact of a dimensional crossover on antiferromagnetic spin correlations and stimulated a renewed interest in low-dimensional quantum many-body physics[17–19].

Other systems to explore the interplay between low-dimensional quantum dynamics and electron correlations are quasi-one-dimensional organic Bechgaard-Fabre salts. A rich variety of phenomena in their global temperature-pressure phase diagram has been ascribed to an increase in electronic dimensionality with applied pressure which triggers a metal-insulator transition[11]. Whether the nature of this higher-dimensional metallic phase and its low-energy excitations can be accounted for by a Fermi liquid theory is the key question in the physics of these compounds.

2 The Hubbard Model and the Quantum Monte Carlo Method

A simple model of various correlated electron systems is the Hubbard model. It captures the essence of nontrivial phenomena which are due to the interplay between the kinetic and potential energy. In one dimension, the Bethe ansatz solution and the bosonization approach have lead to a thorough understanding of the low-energy physics[13]. In higher dimensions, however, rigorous results are scarce. Thus, it is natural to ask the question how the crossover from one to two or higher dimensions takes place. Such a dimensional crossover can be studied by smoothly increasing the hopping amplitude between the individual one-dimensional Hubbard chains. To this end, we consider the Hubbard model on a square lattice with an anisotropic hopping at half-filling (one electron per site),

$$H - \mu N = -\sum_{\boldsymbol{ij},\sigma} t_{\boldsymbol{ij}} c^{\dagger}_{\boldsymbol{i}\sigma} c_{\boldsymbol{j}\sigma} + U \sum_{\boldsymbol{i}} n_{\boldsymbol{i}\uparrow} n_{\boldsymbol{i}\downarrow} - \mu \sum_{\boldsymbol{i},\sigma} n_{\boldsymbol{i}\sigma}, \tag{1}$$

with a local Coulomb repulsion U and electron hopping amplitudes: $t_{ij} = t$ on the intra-chain bonds, $t_{ij} = t_\perp$ on the interchain bonds, and $t_{ij} = -t_\perp/4$ between next-nearest-neighbour sites on two adjacent chains. The latter is expected to suppress at least partially the tendency towards the onset of low-temperature symmetry-broken states and opens a possibility to study a transition from the one-dimensional Mott insulator to a higher-dimensional metal. To ensure a half-filled band away from the one-dimensional limit, we adjust the chemical potential μ.

The proper treatment of the dimensional crossover requires non-perturbative techniques to deal with the interchain hopping. This becomes clear by considering a half-filled Hubbard chain with the Mott insulating ground state: if one starts with the Mott fixed point, a metal-insulator transition upon increasing the interchain kinetic energy is certainly a non-perturbative phenomenon since the interchain hopping is an irrelevant perturbation (in the sense of Wilson's renormalisation group) of the Mott fixed point.

To handle the full complexity of the problem, we use a finite-temperature implementation of the auxiliary-field QMC algorithm (see Ref. 20 and references therein) which allows one to compute the expectation value of an observable O in the grand-canonical ensemble:

$$\langle O \rangle = \frac{\mathrm{Tr}\left[e^{-\beta(H-\mu N)}O\right]}{\mathrm{Tr}\left[e^{-\beta(H-\mu N)}\right]}. \tag{2}$$

It is based on a path integral formulation of the partition function which maps a quantum system in d spatial dimensions onto a $d+1$-dimensional classical problem with an additional imaginary-time dimension $\beta = 1/T$. The essence of the QMC method is to separate the one-body kinetic term H_t and the two-body Hubbard term H_U with the help of the Trotter decomposition,

$$e^{-\Delta\tau(H_U+H_t)} \simeq e^{-\Delta\tau H_U} e^{-\Delta\tau H_t}. \tag{3}$$

A fixed small discretisation of the temporal axis $\Delta\tau$ introduces an overall controlled systematic error of order $(\Delta\tau)^2$. The simulations reviewed in Sec. 3 were performed for lattice sizes up to 20×20 in the presence of weak frustration and close ($t_\perp/t \lesssim 0.3$) to the one-dimensional limit. Here, the limiting factor is the onset of the negative sign problem which ultimately leads to an exponential scaling of computer time as a function of system size and inverse temperature $\beta = 1/T$.

3 Selected Results

In this section, we summarise our present understanding of dimensional crossover phenomena in strongly anisotropic correlated electron systems such as weakly coupled one-dimensional Hubbard chains, as it emerges from large-scale QMC simulations[17,19]. From the theoretical point of view, the complexity of a dimensional crossover in coupled Hubbard chains comes from single- and two-particle processes generated by the interchain coupling[21]. On the one hand, the crossover in metallic chains is easily induced by the interchain *one-particle* hopping process thus replacing the Luttinger liquid behaviour with a conventional Fermi liquid metal[22]. On the other hand, the Mott gap in a half-filled band makes the problem more difficult due to the enhanced relevance of *two-particle* fluctuations: binding of particle-hole pairs from neighbouring chains generates a finite interchain

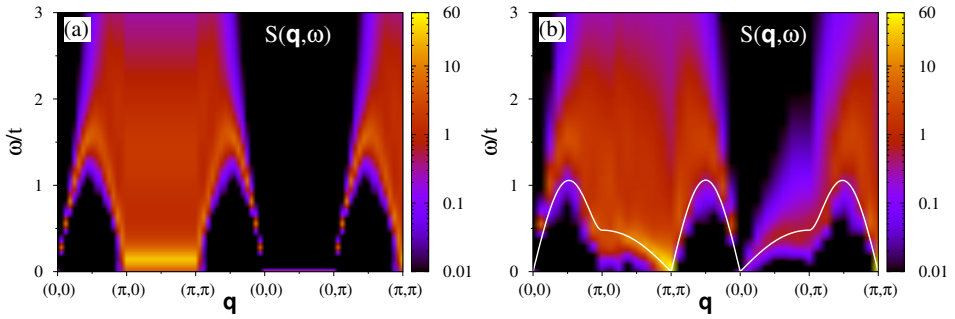

Figure 1. Dimensional-crossover-driven evolution of the magnetic excitation spectrum $S(\boldsymbol{q}, \omega)$ in the effective zero-temperature limit: (a) 32-site Hubbard chain and (b) 16×16 lattice with strong spatial anisotropy $t_\perp/t = 0.3$. The solid line in panel (b) depicts the magnon spectrum obtained within a linear spin-wave theory with the antiferromagnetically ordered ground state. Results taken from Ref. 17.

magnetic interaction $J_\perp$ and may induce an onset of the broken-symmetry phase[23]. In contrast, when the single-particle tunnelling $t_\perp$ overcomes the magnetic coupling $J_\perp$, it drives a metal-insulator transition[24–26].

3.1 Spinon Confinement: Dynamics of Weakly Coupled Hubbard Chains

We begin with the two-particle crossover and a dynamical confinement, a phenomenon mostly known from elementary particle physics. Due to the strong interaction, quarks in a hadron are asymptotically free at a shorter distance and never exist as individual particles. Their condensed-matter counterparts, magnetic quasiparticles (spinons), exhibit similar confinement behaviour. Indeed, in the one-dimensional limit, the magnon excitation which one produces by flipping a spin decomposes into two spinons corresponding to domain walls in the antiferromagnetic background. The spinons can move independently along the chain by subsequent spin flips without cost of energy. Since there is a continuum of ways to distribute the momentum $\boldsymbol{q}$ of the spin-flip process among the two spinons, the corresponding magnetic excitation spectrum is continuous (two-spinon continuum). In the presence of weak interchain interactions, two spinons bind together because their separation would frustrate the interchain bonds. Thus, in analogy with quantum chromodynamics, the interchain interaction plays the role of an attractive potential which grows with the distance between the spinons and confines them back into magnons.

As shown in Fig. 1, lattice QMC simulations allow us to track the evolution of elementary spin excitations upon increasing the coupling between the chains. Our numerical results in the effective zero-temperature limit for the dynamical spin structure factor $S(\boldsymbol{q}, \omega)$ resolve the frequency dependence of the transition from deconfined to confined spinons. In particular, in Fig. 1(b) we identify essentially two frequency regimes dominated by magnetic excitations of different nature: (i) low-frequency magnons, i.e., the Goldstone mode of the broken continuous SU(2) symmetry group, and (ii) intermediate-frequency two-spinon excitations. We interpret this energy-scale separation as follows. Coupling the chains triggers binding of spinons into spin-waves, thereby replacing the low-energy part of the two-spinon continuum depicted in Fig. 1(a). As shown in Fig. 1(b), a simple linear

spin-wave theory with the antiferromagnetically ordered ground state provides quite a good description of the low-energy part of the magnon spectrum along the $(\pi, \pi) \rightarrow (\pi, 0)$ and $(0, 0) \rightarrow (0, \pi)$ paths. However, deconfinement of spinons still occurs above a threshold energy set up by the strength of attractive potential between the spinons. In proximity to the one-dimensional regime, this potential might be easily overcome, explaining the transfer of spectral weight out of the magnon peak into the two-spinon continuum observed at higher frequencies. The simultaneous observation of low-energy *magnons* and high-energy *spinons* is a fingerprint of a magnetically ordered phase coexisting with strong quantum fluctuations brought by reduced dimensionality. Such a dual nature of magnetic excitation spectra has been resolved in the inelastic neutron scattering data on weakly coupled spin-1/2 chains of $KCuF_3$[15].

3.2 Spin and Charge Dynamics of a Quasi-One-Dimensional Antiferromagnetic Metal

In Sec. 3.1 we have presented numerical evidence of the change in the nature of spin excitations on coupling one-dimensional Hubbard chains in the effective zero-temperature limit, where charge fluctuations can be ignored. Here, we discuss a complementary study at finite temperatures where charge fluctuations become progressively more important as a function of the interchain coupling. Consequently, we find the crossover from the one-dimensional Mott phase – which exhibits spin-charge separation – to a higher-dimensional antiferromagnetic metal[19].

A response function particularly suitable for investigating transport properties of anisotropic systems such as weakly coupled Hubbard chains is the frequency- and polarisation-dependent optical conductivity $\sigma_\alpha(\omega)$: it allows one to resolve a distinct behaviour of the charge dynamics along $[\sigma_\parallel(\omega)]$ or perpendicular $[\sigma_\perp(\omega)]$ to the chains. Since the dimensionality is experimentally controlled not only by the physical or chemical pressure, which changes the ratio of interchain to intrachain transfer, but also by the energy scale used in the measurement, the knowledge of $\sigma_\alpha(\omega)$ offers a possibility to track the evolution of remnant aspects of the one-dimensional physics in the high-energy part of the spectrum.

A dimensional-crossover-driven reconstruction of electronic states as evinced by frequency-dependent intrachain $[\sigma_\parallel(\omega)]$ and interchain $[\sigma_\perp(\omega)]$ optical conductivities is shown in Figs. 2(a,b). At our smallest interchain coupling $t_\perp/t = 0.05$, both optical conductivities display solely a finite-frequency feature, as expected for the one-dimensional Mott insulating phase with charge confined to the individual chains. Around $t_\perp/t = 0.15$ a zero-frequency Drude peak in $\sigma_\parallel(\omega)$ develops accompanied by a tiny Drude-like weight in $\sigma_\perp(\omega)$. Given a nearly $t_\perp$-independent position of the finite-frequency absorption and a strongly reduced zero-frequency weight in $\sigma_\perp(\omega)$, the system continues to exhibit a substantial tendency to confine charge carriers. In contrast, a pronounced Drude-like feature in $\sigma_\perp(\omega)$ at larger coupling $t_\perp/t = 0.2$ signals the onset of a higher-dimensional metallic phase with electronic quasiparticles replacing fractionalised excitations characteristic of the one-dimensional regime. Interestingly, most of the optical weight does not form a coherent Drude peak as in a usual Fermi liquid metal, but accumulates at finite frequency thus signalling unconventional charge dynamics.

In order to elucidate the origin of this unconventional behaviour we examine the magnetic excitation spectrum $S(\boldsymbol{q}, \omega)$ at our largest interchain coupling $t_\perp/t = 0.3$ shown in

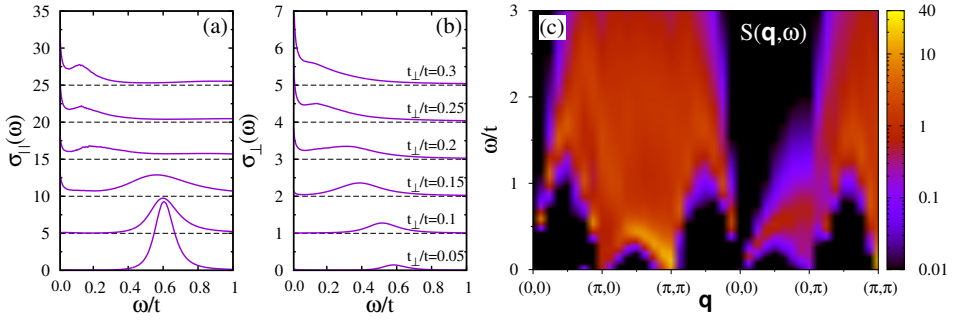

Figure 2. Metal-insulator crossover in weakly coupled one-dimensional Hubbard chains upon increasing the interchain hopping $t_\perp$: (a) intrachain $[\sigma_\parallel(\omega)]$ and (b) interchain $[\sigma_\perp(\omega)]$ optical spectra for a 16×16 lattice at temperature $T = t/20$. From bottom to top: $t_\perp/t = 0.05$, 0.1, 0.15, 0.2, 0.25, and 0.3. Panel (c) shows the magnetic excitation spectrum $S(\boldsymbol{q}, \omega)$ in the metallic phase with short-range antiferromagnetic spin fluctuations at $t_\perp/t = 0.3$. Results taken from Ref. 19.

Fig. 2(c). The most striking difference with respect to the one-dimensional regime is a broad dispersive feature along the $(\pi, \pi) \rightarrow (\pi, 0)$ direction. It is a signature of damped antiferromagnetic spin fluctuations (paramagnons) which are not strong enough to gap out the Fermi surface and develop long-range antiferromagnetic order but nevertheless can propagate an appreciable distance. As indicated by their broad spectral width, these paramagnons have a short lifetime due to scattering off mobile charge carriers and merge into a Fermi-liquid-like particle-hole continuum on moving away from $\boldsymbol{q} = (\pi, \pi)$.

4 Conclusions

We presented a large-scale QMC study of a dimensional crossover in weakly coupled one-dimensional Hubbard chains at half-filling. The simulations allow us to study how the exotic one-dimensional physics relates to a more familiar semiclassical picture valid in higher-dimensional systems. In particular, the evolution of the dynamical spin structure factor upon increasing the interchain coupling in the effective zero-temperature limit indicates a change in the nature of elementary spin excitations from a two-spinon continuum to low-energy spin-waves. Furthermore, finite-temperature results provide evidence of the crossover from the one-dimensional Mott phase to a higher-dimensional antiferromagnetic metal. We have placed emphasis on clarifying the nature of this metallic phase and its low-energy excitations. Our simulations provide a deeper understanding of the intricate spin and charge dynamics of low-dimensional correlated electron systems.

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References

1. D. J. Luitz, F. F. Assaad, T. Novotný, C. Karrasch, and V. Meden, *Understanding the Josephson Current through a Kondo-Correlated Quantum Dot*, Phys. Rev. Lett., **108**, 227001, 2012.
2. M. Hohenadler, F. Parisen Toldin, I. F. Herbut, and F. F. Assaad, *Phase diagram of the Kane-Mele-Coulomb model*, Phys. Rev. B, **90**, 085146, 2014.
3. F. F. Assaad and T. C. Lang, *Diagrammatic determinantal quantum Monte Carlo methods: Projective schemes and applications to the Hubbard-Holstein model*, Phys. Rev. B, **76**, 035116, 2007.
4. M. Weber, F. F. Assaad, and M. Hohenadler, *Excitation spectra and correlation functions of quantum Su-Schrieffer-Heeger models*, Phys. Rev. B, **91**, 245147, 2015.
5. M. Weber, F. F. Assaad, and M. Hohenadler, *Excitation spectra and correlation functions of quantum Su-Schrieffer-Heeger models*, Phys. Rev. B, **91**, 245147, 2015.
6. F. F. Assaad and I. F. Herbut, *Pinning the Order: The Nature of Quantum Criticality in the Hubbard Model on Honeycomb Lattice*, Phys. Rev. X, **3**, 031010, 2013.
7. F. Parisen Toldin, M. Hohenadler, F. F. Assaad, and I. F. Herbut, *Fermionic quantum criticality in honeycomb and π-flux Hubbard models: Finite-size scaling of renormalization-group-invariant observables from quantum Monte Carlo*, Phys. Rev. B, **91**, 165108, 2015.
8. M. Hohenadler and F. F. Assaad, *Rashba coupling and magnetic order in correlated helical liquids*, Phys. Rev. B, **90**, 245148, 2014.
9. M. Bercx, M. Hohenadler, and F. F. Assaad, *Kane-Mele-Hubbard model on the π-flux honeycomb lattice*, Phys. Rev. B, **90**, 075140, 2014.
10. E. W. Carlson, D. Orgad, S. A. Kivelson, and V. J. Emery, *Dimensional crossover in quasi-one-dimensional and high-T_c superconductors*, Phys. Rev. B, **62**, 3422, 2000.
11. V. Vescoli, L. Degiorgi, W. Henderson, G. Grüner, K. Starkey, and L. K. Montgomery, *Dimensionality-Driven Insulator-to-Metal Transition in the Bechgaard Salts.*, Science, **281**, 1181, 1998.
12. A. Auerbach, *Interacting Electrons and Quantum Magnetism*, Springer-Verlag, New York, 1994.
13. T. Giamarchi, *Quantum Physics in One Dimension*, Oxford University, Oxford, 2004.
14. B. Lake, A. M. Tsvelik, S. Notbohm, D. A. Tennant, T. G. Perring, M. Reehuis, C. Sekar, G. Krabbes, and B. Büchner, *Confinement of fractional quantum number particles in a condensed-matter system*, Nat. Phys., **6**, 50, 2010.
15. B. Lake, D. A. Tennant, C. D. Frost, and S. E. Nagler, *Quantum criticality and universal scaling of a quantum antiferromagnet*, Nat. Mater., **4**, 329, 2005.
16. D. Greif, T. Uehlinger, G. Jotzu, L. Tarruell, and T. Esslinger, *Short-Range Quantum Magnetism of Ultracold Fermions in an Optical Lattice*, Science, **340**, 1307, 2013.
17. M. Raczkowski and F. F. Assaad, *Spinon confinement: Dynamics of weakly coupled Hubbard chains*, Phys. Rev. B, **88**, 085120, 2013.

18. J. Imriška, M. Iazzi, L. Wang, E. Gull, D. Greif, T. Uehlinger, G. Jotzu, L. Tarruell, T. Esslinger, and M. Troyer, *Thermodynamics and Magnetic Properties of the Anisotropic 3D Hubbard Model*, Phys. Rev. Lett., **112**, 115301, 2014.
19. M. Raczkowski, F. F. Assaad, and L. Pollet, *Spin and charge dynamics of a quasi-one-dimensional antiferromagnetic metal*, Phys. Rev. B, **91**, 045137, 2015.
20. F. Assaad and H. Evertz, "World-line and determinantal quantum monte carlo methods for spins, phonons and electrons", in: Computational Many-Particle Physics, H. Fehske, R. Schneider, and A. Weiße, (Eds.), vol. 739 of *Lecture Notes in Physics*, pp. 277–356. Springer, Berlin Heidelberg, 2008.
21. A. O. Gogolin, A. A. Nersesyan, and A. M. Tsvelik, *Bosonization and Strongly Correlated Systems*, Cambridge University Press, Cambridge, 2004.
22. C. Castellani, C. Di Castro, and W. Metzner, *Dimensional crossover from Fermi to Luttinger liquid*, Phys. Rev. Lett., **72**, 316, 1994.
23. I. Affleck and B. I. Halperin, *On a renormalization group approach to dimensional crossover*, J. Phys. A: Math. Gen., **29**, 2627, 1996.
24. S. Biermann, A. Georges, A. Lichtenstein, and T. Giamarchi, *Deconfinement Transition and Luttinger to Fermi Liquid Crossover in Quasi-One-Dimensional Systems*, Phys. Rev. Lett., **87**, 276405, 2001.
25. F. H. L. Essler and A. M. Tsvelik, *Weakly coupled one-dimensional Mott insulators*, Phys. Rev. B, **65**, 115117, 2002.
26. M. Raczkowski and F. F. Assaad, *Dimensional-Crossover-Driven Mott Transition in the Frustrated Hubbard Model*, Phys. Rev. Lett., **109**, 126404, 2012.